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NuMa-Report No. 2017-03

May 2017

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Multipatch Space-Time Isogeometric Analysis of Parabolic Diffusion Problems

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Abstract. We present and analyze a new stable multi-patch space-time Isogeometric Analysis (IgA) method for the numerical solution of parabolic diffusion problems. The discrete bilinear form is elliptic on the IgA space with respect to a mesh-dependent energy norm. This property together with a corresponding boundedness property, consistency and approximation results for the IgA spaces yields a priori discretization error estimates. We propose an efficient implementation technique via tensor product representation, and fast space-time parallel solvers. We present numerical results confirming the efficiency of the space-time solvers on massively parallel computers using more than 100.000 cores.

Keywords: Parabolic initial-boundary value problems, space-time isogeometric analysis, a priori discretization error estimates, parallel solvers.

1 Introduction

The standard discretization methods for parabolic initial-boundary value problems (IBVP) are based on a separation of the discretizations in space and time, i.e., first space, then time, or, vice versa, first time, then space. The former one is called vertical method of lines, whereas the latter one is called horizontal method of lines or Rothe's method. Both methods use some kind of time-stepping method for time discretization. This is a sequential procedure that needs some smart ideas for the parallelization with respect to time, see [5] for a historical overview of time-parallel methods. Other disadvantages of these approaches are connected with a separation of adaptivity with respect to space and time, and with difficulties in the numerical treatment of moving interfaces and spatial domains. To overcome this curse of sequentiality of time-stepping methods, one should look at the time variable t as just another variable, say, x_{d+1} if x_1, \dots, x_d are the spatial variable, and at the time derivative as a strong convection in the direction x_{d+1} . In [11], we were inspired by this view at parabolic problems, and proposed upwind-stabilized single-patch space-time IgA schemes for parabolic evolution problems. For comprehensive overview on the literature on different space-time methods for solving parabolic IPVP, we also refer to [11].

In this paper, we generalize the results of [11] from the single-patch to the time dG multi-patch IgA case. As in [11], we consider the linear parabolic IBVP: find $u : \overline{Q} \rightarrow \mathbb{R}$ such that

$$\partial_t u - \Delta u = f \text{ in } Q, \quad u = 0 \text{ on } \Sigma, \quad \text{and } u = u_0 \text{ on } \Sigma_0, \quad (1)$$

as a typical model problem posed in the space-time cylinder $\overline{Q} = \overline{\Omega} \times [0, T] = Q \cup \Sigma \cup \overline{\Sigma}_0 \cup \overline{\Sigma}_T$, where ∂_t denotes the partial time derivative, Δ is the Laplace operator, f is a given source function, u_0 are the given initial data, T is the final time, $Q = \Omega \times (0, T)$, $\Sigma = \partial\Omega \times (0, T)$, $\Sigma_0 := \Omega \times \{0\}$, $\Sigma_T := \Omega \times \{T\}$, and $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) denotes the spatial computational domain with the boundary $\partial\Omega$. The spatial domain Ω is supposed to be bounded and Lipschitz. Later we will assume that Ω has a single- or multipatch NURBS representation as is used in CAD respectively IgA.

2 Space-time variational formulation

Using the standard procedure and integration by parts with respect to both x and t , we can easily derive the following space-time variational formulation of (1): find $u \in H_0^{1,0}(Q) = \{u \in L_2(Q) : \nabla_x u \in [L_2(Q)]^d, u = 0 \text{ on } \Sigma\}$ such that

$$a(u, v) = l(v), \quad \forall v \in H_{0,0}^{1,1}(Q), \quad (2)$$

with the bilinear form

$$a(u, v) = - \int_Q u(x, t) \partial_t v(x, t) dx dt + \int_Q \nabla_x u(x, t) \cdot \nabla_x v(x, t) dx dt \quad (3)$$

and the linear form

$$l(v) = \int_Q f(x, t) v(x, t) dx dt + \int_{\Omega} u_0(x) v(x, 0) dx, \quad (4)$$

where $H_{0,0}^{1,1}(Q) = \{u \in L_2(Q) : \nabla_x u \in [L_2(Q)]^d, \partial_t u \in L_2(Q), u = 0 \text{ on } \Sigma, \text{ and } u = 0 \text{ on } \Sigma_T\}$. The space-time variational formulation (2) has a unique solution, see, e.g., [9,10]. In these monographs, beside existence and uniqueness results, one can also find useful a priori estimates and regularity results. For simplicity, we below assume that $u_0 = 0$.

3 Stable multi-patch space-time IgA discretization

Let us now assume that the space-time cylinder $\overline{Q} = \cup_{n=1}^N \overline{Q}_n$ consists of N subcylinders (patches or time slices) $Q_n = \Omega \times (t_{n-1}, t_n)$, $n = 1, \dots, N$, where $0 = t_0 < t_1 < \dots < t_N = T$ is some subdivision of time interval $[0, T]$. The time faces between the time patches are denoted by $\overline{\Sigma}_n = \overline{Q}_{n+1} \cap \overline{Q}_n = \overline{\Omega} \times \{t_n\}$. We obviously have $\Sigma_N = \Sigma_T$. Every space-time patch $Q_n = \Phi_n(\hat{Q})$ in the

physical domain Q can be represented as the image of the parameter domain $\widehat{Q} = (0, 1)^{d+1}$ by means of a sufficiently regular IgA (B-Spline, NURBS etc.) map $\Phi_n : \widehat{Q} \rightarrow Q_n$, i.e.,

$$\Phi_n(\xi) = \sum_{i \in \mathcal{I}_n} \mathbf{P}_{n,i} \widehat{\varphi}_{n,i}(\xi), \quad (5)$$

where $\{\widehat{\varphi}_{n,i}\}_{i \in \mathcal{I}_n}$ are the IgA basis functions, and $\{\mathbf{P}_{n,i}\}_{i \in \mathcal{I}_n} \subset \mathbb{R}^{d+1}$ are the control points for the patch Q_n . The IgA basis functions are usually multivariant B-Splines or NURBS defined on a mesh given by the knot vector wrt to each direction in the parameter domain \widehat{Q} , and the underlying polynomial degrees and multiplicities of the knots defining the smoothnesses of the basis functions, see, e.g., [2] or [12] for more detailed information.

Now, we can construct our finite-dimensional IgA (B-Spline, NURBS etc.) space $V_{0h} = \{v_h : v_n = v_h|_{Q_n} \in V_{0n}, n = 1, \dots, N\}$, the functions of which are smooth in each time patch Q_n in correspondence to the smoothness of the splines, but in general discontinuous across the time faces $\Sigma_n, n = 1, \dots, N-1$. The smooth IgA spaces $V_{0n} = V_{0h_n} = \text{span}\{\varphi_{n,i}\}_{i \in \mathcal{I}_n} \subset H_0^{1,1}(Q_n)$ are spanned by IgA basis functions $\{\varphi_{n,i}\}_{i \in \mathcal{I}_n}$ that are nothing but the images of the basis functions $\{\widehat{\varphi}_{n,i}\}_{i \in \mathcal{I}_n}$, which were already used for defining the patch Q_n , by the map Φ_n , i.e., $\varphi_{n,i} = \widehat{\varphi}_{n,i} \circ \Phi_n^{-1}$. The basis functions $\varphi_{1,i}$ should vanish on Σ_0 for all $i \in \mathcal{I}_1$. Therefore, all functions v_h from V_{0h} fulfil homogeneous boundary and initial conditions. The discretization parameter h_n denotes the average mesh-size of the mesh induced by the corresponding mesh in the parameter domain \widehat{Q} via the map Φ_n . The IgA technology of using the same basis functions for describing the patches of the computational domain (geometry) and for defining the approximation spaces V_{0h} was introduced by Hughes, Cottrell and Bazilevs in 2005 [8] and analyzed in [1], see also monograph [2] for more comprehensive information.

In order to derive our dG IgA scheme for defining the IgA solution $u_h \in V_{0h}$, we multiply the parabolic PDE (1) by a time-upwind test function of the form $v_n + \theta_n h_n \partial_t v_n$ with an arbitrary $v_n \in V_{0n}$ and a positive, sufficiently small constant θ_n , and integrate over the space-time subcylinder Q_n . After integration by parts wrt x , we get

$$\begin{aligned} & \int_{Q_n} (\partial_t u(v_n + \theta_n h_n \partial_t v_n) + \nabla_x u \cdot \nabla_x v_n + \theta_n h_n \nabla_x u \cdot \nabla_x \partial_t v_n) dx dt \\ & - \int_{\partial Q_n} \mathbf{n}_x \cdot \nabla_x u (v_n + \theta_n h_n \partial_t v_n) ds = \int_{Q_n} f(v_n + \theta_n h_n \partial_t v_n) dx dt. \end{aligned} \quad (6)$$

We mention that $\partial_t v_n$ is differentiable wrt x due to the special tensor product structure of V_{0n} . Using the facts that v_n and $\partial_t v_n$ are always zero on Σ , and the x -components $\mathbf{n}_x = (n_1, \dots, n_d)^\top$ of the normal $\mathbf{n} = (n_1, \dots, n_d, n_{d+1})^\top = (\mathbf{n}_x, n_t)^\top$ are zero on Σ_{n-1} and Σ_n , we observe that the integral over ∂Q_n is always zero. Now, adding to the left-hand side of (6) a consistent time-upwind

term for stabilization, and summing over all time patches, we get the identity

$$\begin{aligned} & \sum_{n=1}^N \int_{Q_n} (\partial_t u(v_n + \theta_n h_n \partial_t v_n) + \nabla_x u \cdot \nabla_x v_n + \theta_n h_n \nabla_x u \cdot \nabla_x \partial_t v_n) dx dt \\ & + \sum_{n=1}^N \int_{\Sigma_{n-1}} [[u]] v_n dx = \sum_{n=1}^N \int_{Q_n} f(v_n + \theta_n h_n \partial_t v_n) dx dt \end{aligned} \quad (7)$$

that holds for a sufficiently smooth solution u of our parabolic IBVP, where $[[u]] := u|_{Q_n} - u|_{Q_{n-1}}$ on Σ_{n-1} denotes the jump of u across Σ_{n-1} that is obviously zero.

The time multipatch space-time IgA scheme for solving the parabolic IBVP (1) respectively (2) can now be formulated as follows: find $u_h \in V_{0h}$ such that

$$a_h(u_h, v_h) = l_h(v_h), \quad \forall v_h \in V_{0h}, \quad (8)$$

where

$$\begin{aligned} a_h(u_h, v_h) &= \sum_{n=1}^N a_n(u_h, v_h) = \sum_{n=1}^N \left(\int_{Q_n} (\partial_t u_n(v_n + \theta_n h_n \partial_t v_n) + \nabla_x u_n \cdot \nabla_x v_n \right. \\ & \quad \left. + \theta_n h_n \nabla_x u_n \cdot \nabla_x \partial_t v_n) dx dt + \int_{\Sigma_{n-1}} [[u_h]] v_n dx \right), \end{aligned} \quad (9)$$

$$l_h(v_h) = \sum_{n=1}^N l_n(v_h) = \sum_{n=1}^N \int_{Q_n} f(v_n + \theta_n h_n \partial_t v_n) dx dt. \quad (10)$$

Here and below we formally set $[[u_1]]$ on Σ_0 to zero since we assumed homogeneous initial conditions. It is clear that this jump term can be used to include inhomogeneous initial conditions in a weak sense. In this case, the test functions v_n are not forced to be zero on Σ_0 . The derivation of the IgA scheme given above immediately yields that this scheme is consistent for sufficiently smooth solution, cf. identity (7). Indeed, if the solution $u \in H_0^{1,0}(Q)$ of (2) belongs to $H_0^{1,1}(Q)$, then it satisfies the consistency identity

$$a_h(u, v_h) = l_h(v_h), \quad \forall v_h \in V_{0h}, \quad (11)$$

yielding Galerkin orthogonality

$$a_h(u - u_h, v_h) = 0, \quad \forall v_h \in V_{0h}. \quad (12)$$

Now we will show that the bilinear form $a_h(\cdot, \cdot)$ is V_{0h} -elliptic wrt the norm $\|v\|_h$ defined by

$$\|v\|_h^2 = \sum_{n=1}^N \left(\frac{1}{2} \|\nabla_x v\|_{L_2(Q_n)}^2 + \theta_n h_n \|\partial_t v\|_{L_2(Q_n)}^2 + \frac{1}{2} \|[[v]]\|_{L_2(\Sigma_{n-1})}^2 \right) + \frac{1}{2} \|v\|_{L_2(\Sigma_N)}^2.$$

In order to show the V_{0h} -ellipticity of $a_h(\cdot, \cdot)$, we need the inverse inequality

$$\|\nabla_x v_n\|_{L_2(\Sigma_{n-1})}^2 \leq c_{inv,0}^2 h_n^{-1} \|\nabla_x v_n\|_{L_2(Q_n)}^2 \quad (13)$$

that is valid for all $v_n \in V_{0n}$ and $n = 1, \dots, N$, see [1,4].

Lemma 1. *The bilinear form $a_h(\cdot, \cdot)$ defined by (9) is V_{0h} -elliptic, i.e., there exist a generic positive constant μ_e such that*

$$a_h(v_h, v_h) \geq \mu_e \|v_h\|_h^2, \quad \forall v_h \in V_{0h}. \quad (14)$$

provided that the parameters θ_n are sufficiently small. More precisely, $\mu_e = 1$ if $0 < \theta_n \leq c_{inv,0}^{-2}$ for all $n = 1, 2, \dots, N$, where $c_{inv,0}$ is the constant from the inverse inequality (13).

Proof. Using integration by parts with respect to t and the inverse inequality (13), we can derive the following estimates:

$$\begin{aligned} a_n(v_h, v_h) &= \int_{Q_n} \left(\frac{1}{2} \partial_t v_n^2 + \theta_n h_n (\partial_t v_n)^2 + |\nabla_x v_n|^2 + \frac{\theta_n h_n}{2} \partial_t |\nabla_x v_n|^2 \right) dx dt \\ &\quad + \int_{\Sigma_{n-1}} [|v_h|] v_n dx \\ &= \frac{1}{2} \int_{\Sigma_n} v_n^2 dx - \frac{1}{2} \int_{\Sigma_{n-1}} v_n^2 dx + \int_{Q_n} (\theta_n h_n (\partial_t v_n)^2 + |\nabla_x v_n|^2) dx dt \\ &\quad + \frac{\theta_n h_n}{2} \int_{\Sigma_n} |\nabla_x v_n|^2 dx - \frac{\theta_n h_n}{2} \int_{\Sigma_{n-1}} |\nabla_x v_n|^2 dx + \int_{\Sigma_{n-1}} [|v_h|] v_n dx \\ &\geq \theta_n h_n \|\partial_t v_n\|_{L_2(Q_n)}^2 + \|\nabla_x v_n\|_{L_2(Q_n)}^2 - 0.5 \theta_n h_n \|\nabla_x v_n\|_{L_2(\Sigma_{n-1})}^2 \\ &\quad + \frac{1}{2} \int_{\Sigma_n} v_n^2 dx - \frac{1}{2} \int_{\Sigma_{n-1}} v_n^2 dx + \int_{\Sigma_{n-1}} v_n^2 dx - \int_{\Sigma_{n-1}} v_{n-1} v_n dx \\ &\geq \theta_n h_n \|\partial_t v_n\|_{L_2(Q_n)}^2 + (1 - 0.5 \theta_n c_{inv,0}^2) \|\nabla_x v_n\|_{L_2(Q_n)}^2 \\ &\quad + \int_{\Sigma_{n-1}} \left(\frac{1}{2} v_n^2 - v_{n-1} v_n \right) dx + \frac{1}{2} \int_{\Sigma_n} v_n^2 dx \end{aligned}$$

Summing over all $n = 1, \dots, N$, we obtain

$$\begin{aligned} a_h(v_h, v_h) &= \sum_{n=1}^N a_n(v_h, v_h) \\ &\geq \sum_{n=1}^N \theta_n h_n \|\partial_t v_h\|_{L_2(Q_n)}^2 + (1 - 0.5 \theta_n c_{inv,0}^2) \|\nabla_x v_h\|_{L_2(Q_n)}^2 \\ &\quad + \sum_{n=1}^N \frac{1}{2} \|[v_h]\|_{L_2(\Sigma_{n-1})}^2 + \frac{1}{2} \|v_N\|_{L_2(\Sigma_N)}^2. \end{aligned}$$

Choosing $0 < \theta_n \leq c_{inv,0}^{-2}$ for all $n = 1, 2, \dots, N$, we immediately arrive at (14) with $\mu_e = 1$. ■

Lemma 1 immediately implies that the solution $u_h \in V_{0h}$ of (8) is unique. Since the IgA scheme (8) is posed in the finite dimensional space V_{0h} , the uniqueness yields existence of the solution $u_h \in V_{0h}$ of (8).

Once the basis is chosen, the IgA scheme (8) can be rewritten as a huge linear system of algebraic equations of the form

$$\mathbf{L}_h \mathbf{u}_h = \mathbf{f}_h \quad (15)$$

for determining the vector $\mathbf{u}_h = ((u_{1,i})_{i \in \mathcal{I}_1}, \dots, (u_{N,i})_{i \in \mathcal{I}_N}) \in \mathbb{R}^{N_h}$ of the control points of the IgA solution

$$u_h(x, t) = \sum_{i \in \mathcal{I}_n} u_{n,i} \varphi_{n,i}(x, t), \quad (x, t) \in \bar{Q}_n, \quad n = 1, \dots, N, \quad (16)$$

solving the IgA scheme (8). The system matrix \mathbf{L}_h is the usual Galerkin (stiffness) matrix, and \mathbf{f}_h is the corresponding right-hand side (load) vector.

4 A priori discretization error estimates

In order to derive a priori discretization error estimates, we will first show that the IgA bilinear form $a_h(\cdot, \cdot)$ is bounded on $V_{0h,*} \times V_{0h}$, where the space $V_{0h,*} = V + V_{0h}$ is equipped with the norm $\|\cdot\|_{h,*}$ defined by the relation

$$\|v\|_{h,*}^2 = \|v\|_h^2 + \sum_{n=1}^N (\theta_n h_n)^{-1} \|v\|_{L_2(Q_n)}^2 + \sum_{n=2}^N \|v|_{Q_n}\|_{L_2(\Sigma_{n-1})}^2, \quad (17)$$

and V is a suitable infinite-dimensional space containing the solution u , e.g., we can choose $V = H_{0,\underline{0}}^{1,1}(Q) = \{u \in L_2(Q) : \nabla_x u \in [L_2(Q)]^d, \partial_t u \in L_2(Q), u = 0 \text{ on } \Sigma, \text{ and } u = 0 \text{ on } \Sigma_0\}$ assuming that the solution u belongs to this space. In order to prove the boundedness of $a_h(\cdot, \cdot)$, we need the inverse inequality

$$\|\nabla_x \partial_t v_n\|_{L_2(Q_n)}^2 \leq c_{inv,1}^2 h_n^{-2} \|\nabla_x v_n\|_{L_2(Q_n)}^2 \quad (18)$$

that is valid for all $v_n \in V_{0n}$ and $n = 1, \dots, N$, see [1,4].

Lemma 2. *The bilinear form $a_h(\cdot, \cdot)$ defined by (9) is bounded on the space $V_{0h,*} \times V_{0h}$, i.e., there exists a generic positive constant μ_b such that*

$$|a_h(u, v_h)| \leq \mu_b \|u\|_{h,*} \|v_h\|_h, \quad \forall u \in V_{0h,*}, \quad \forall v_h \in V_{0h}. \quad (19)$$

with the boundedness constant $\mu_b = 2 \max\{\sqrt{1 + c_{inv,1}^2/c_{inv,0}^2}, \sqrt{2}\}$, where $c_{inv,0}$ and $c_{inv,1}$ are the constants from inequalities (13) and (18). We always assume that the parameters θ_n are chosen as in Lemma 1.

Proof. For the first and the interface jump terms of a_h , we use Green's formula and the Cauchy inequality to derive the following estimates:

$$\begin{aligned}
& \sum_{n=1}^N \left(\int_{Q_n} \partial_t u v_h \, dx \, dt + \int_{\Sigma_{n-1}} [|u|] v_n \, ds \right) \\
&= \sum_{n=1}^N \left(- \int_{Q_n} u \partial_t v_h \, dx \, dt + \int_{\Sigma_n} u v_n \, ds - \int_{\Sigma_{n-1}} u v_n \, ds + \int_{\Sigma_{n-1}} [|u|] v_n \, ds \right) \\
&\leq \left(\sum_{n=1}^N (\theta_n h_n)^{-1} \left(\int_{Q_n} u^2 \, dx \, dt \right)^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^N \theta_n h_n \left(\int_{Q_n} (\partial_t v_n)^2 \, dx \, dt \right)^2 \right)^{\frac{1}{2}} \\
&\quad + \sum_{n=1}^N \int_{\Sigma_{n-1}} (v_{n-1} - v_n) u \, ds + \int_{\Sigma_N} v_n u \, ds \\
&\leq \left(\sum_{n=1}^N (\theta_n h_n)^{-1} \left(\int_{Q_n} u^2 \, dx \, dt \right)^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^N \theta_n h_n \left(\int_{Q_n} (\partial_t v_n)^2 \, dx \, dt \right)^2 \right)^{\frac{1}{2}} \\
&\quad + \sqrt{2} \left(\frac{1}{2} \sum_{n=1}^N \|v_h\|_{L^2(\Sigma_{n-1})}^2 + \frac{1}{2} \|v_N\|_{L^2(\Sigma_N)}^2 \right)^{\frac{1}{2}} \sqrt{2} \left(\sum_{n=1}^N \|u\|_{L^2(\Sigma_{n-1})}^2 + \frac{1}{2} \|u\|_{L^2(\Sigma_N)}^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

Using again Cauchy's inequality, we get the estimates

$$\begin{aligned}
& \sum_{n=1}^N \int_{Q_n} (\theta_n h_n)^{\frac{1}{2}} \partial_t u (\theta_n h_n)^{\frac{1}{2}} \partial_t v_n \, dx \, dt + \sum_{n=1}^N \int_{Q_n} \nabla_x u \cdot \nabla_x v_n \, dx \, dt \\
&\leq \left(\sum_{n=1}^N \theta_n h_n \|\partial_t u\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^N \theta_n h_n \|\partial_t v_n\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \\
&\quad + \sqrt{2} \left(\frac{1}{2} \sum_{n=1}^N \|\nabla_x u\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \sqrt{2} \left(\frac{1}{2} \sum_{n=1}^N \|\nabla_x v_n\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}}
\end{aligned}$$

for the second and third terms. Finally, for the last but one term, we apply Cauchy's and inverse inequalities to show

$$\begin{aligned}
& \sum_{n=1}^N \int_{Q_n} \nabla_x u \cdot (\theta_n h) \nabla_x \partial_t v_n \, dx \, dt \\
&\leq \left(\sum_{n=1}^N \|\nabla_x u\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^N (\theta_n h_n)^2 \|\nabla_x \partial_t v_n\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \\
&\leq \left(\sum_{n=1}^N \|\nabla_x u\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \left(\sum_{n=1}^N (\theta_n h_n)^2 c_{inv,1}^2 h_n^{-2} \|\nabla_x v_n\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \\
&\leq c_{inv,1} \theta_n \sqrt{2} \left(\frac{1}{2} \sum_{n=1}^N \|\nabla_x u\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}} \sqrt{2} \left(\frac{1}{2} \sum_{n=1}^N \|\nabla_x v_n\|_{L^2(Q_n)}^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

Gathering together the bounds obtained above yields estimate (19) with $\mu_b = 2 \max\{\sqrt{1 + c_{inv,1}\theta}, \sqrt{2}\}$, where $\theta = \max_{n=1,\dots,N}\{\theta_n\} \leq c_{inv,0}^{-2}$. \blacksquare

Let v_h be an arbitrary IgA function from V_{h0} . Using the fact that $v_h - u_h \in V_{h0}$, the V_{h0} -ellipticity of the bilinear form $a_h(\cdot, \cdot)$ as was shown in Lemma 1, the Galerkin orthogonality (12), and the boundedness (19) of $a_h(\cdot, \cdot)$ on $V_{0h,*} \times V_{0h}$, we can derive the following estimate

$$\begin{aligned} \mu_e \|v_h - u_h\|_h^2 &\leq a_h(v_h - u_h, v_h - u_h) = a_h(v_h - u, v_h - u_h) \\ &\leq \mu_b \|v_h - u\|_{h,*} \|v_h - u_h\|_h. \end{aligned}$$

Therefore, we can proceed as follows:

$$\begin{aligned} \|u - u_h\|_h &\leq \|u - v_h\|_h + \|v_h - u_h\|_h \\ &\leq \|u - v_h\|_h + (\mu_b/\mu_e) \|v_h - u\|_{h,*} \\ &\leq (1 + \mu_b/\mu_e) \|v_h - u\|_{h,*}, \end{aligned}$$

which proves the following Cea-like Lemma providing an estimate of the discretization error wrt the norm $\|\cdot\|_h$ by the best approximation error wrt to the $\|\cdot\|_{h,*}$ norm.

Lemma 3. *Under the assumption made above, the discretization error wrt the $\|\cdot\|_h$ norm can be estimated from above by the best approximation error wrt to the $\|\cdot\|_{h,*}$ norm as follows:*

$$\|u - u_h\|_h \leq (1 + \frac{\mu_b}{\mu_e}) \inf_{v_h \in V_{0h}} \|u - v_h\|_{h,*}. \quad (20)$$

Theorem 1. *Let the solution $u \in H_0^{1,0}(Q)$ of the parabolic initial-boundary value model problem (2) belong to $V = H_{0,0}^{1,1}(Q)$ globally, and patch-wise to $H^{s_n}(Q_n)$ with some $s_n \geq 2$ for $n = 1, \dots, N$, and let $u_h \in V_{0h}$ be the solution to the IgA scheme (8) with fixed positive θ_n , $n = 1, \dots, N$, defined as in Lemma 1. Then the discretization error estimate*

$$\|u - u_h\|_h \leq (1 + \frac{\mu_b}{\mu_e}) \sum_{n=1}^N c_n h_n^{r_n-1} \|u\|_{H^{r_n}(Q_n)} \quad (21)$$

holds, where c_n are generic positive constants, $r_n = \min\{s_n, p_n + 1\}$, and p_n denotes the underlying polynomial degree of the B-splines or NURBS used in patch Q_n with $n = 1, \dots, N$.

Proof. Let Π_n be a projective operator from $L_2(Q_n)$ to V_{0n} that delivers optimal approximation error estimates in the $L_2(Q_n)$ and $H^1(Q_n)$ norms, see, e.g., [1] or [3]. We define the multi-patch projective operator $(\Pi_h u)|_{Q_n} = \Pi_n(u|_{Q_n})$ for all $n = 1, \dots, N$. Employing the approximation results given in [1] or [3], we can easily derive the approximation error estimates

$$\|\nabla_x(u - \Pi_h u)\|_{L^2(Q_n)}^2 + \theta_n h_n \|\partial_t(u - \Pi_h u)\|_{L^2(Q_n)}^2 \leq C_1 h_n^{2(r_n-1)} \|u\|_{H^{r_n}(Q_n)}^2 \quad (22)$$

and

$$\theta_n h_n^{-1} \|u - \Pi_n u\|_{L^2(Q_n)}^2 \leq C_2 h_n^{2r_n-1} \|u\|_{H^{r_n}(Q_n)}^2, \quad (23)$$

with positive generic constants C_1 and C_2 . Based on the previous estimates and the trace inequality

$$\|u\|_{L^2(\partial Q_n)}^2 \leq C_{tr} h_n^{-1} (\|u\|_{L^2(Q_n)}^2 + h_n^2 \|u\|_{H^1(Q_n)}^2),$$

we can further show the approximation error estimate

$$\|u - \Pi_n u\|_{L^2(\partial Q_n)}^2 \leq C_3 h^{2r_n-1} \|u\|_{H^{r_n}(Q_n)}^2$$

that in turn implies

$$\|u - \Pi_n u\|_{L^2(\Sigma_n)}^2 \leq C_4 h^{2r_n-1} \|u\|_{H^{r_n}(Q_n)}^2 \quad (24)$$

and

$$\begin{aligned} \frac{1}{2} \| [u - \Pi_h u] \|_{L^2(\Sigma_{n-1})}^2 &\leq \|u_n - \Pi_n u\|_{L^2(\Sigma_{n-1})}^2 + \|u_{n-1} - \Pi_{n-1} u\|_{L^2(\Sigma_{n-1})}^2 \\ &\leq C_4 h_n^{2r_n-1} \|u\|_{H^{r_n}(Q_n)}^2 + C_5 h_{n-1}^{2r_{n-1}-1} \|u\|_{H^{r_{n-1}}(Q_{n-1})}^2, \end{aligned} \quad (25)$$

with positive generic constants C_4 and C_5 . Finally, gathering together (22), (23), (24) and (25), summing over all space-time patches Q_n , and recalling definition (17), we get the approximation error estimate

$$\|u - \Pi_h u\|_{h,*} \leq \sum_{n=1}^N c_n h_n^{r_n-1} \|u\|_{H^{r_n}(Q_n)}. \quad (26)$$

Inserting (26) into (20) yields the desired result. \blacksquare

Remark 1. The above estimate has been derived under the isotropic assumption $u \in H^{s_n}(Q_n)$ for the patch-wise regularity of the solution. In the forthcoming work [7], we will present a discretization error analysis for the case when the solution can have anisotropic regularity behavior with respect to time and space.

5 Matrix representation and space-time multigrid solvers

We now assume that the IgA map $\Phi_n : \widehat{Q} \rightarrow Q_n$ preserves the tensor product structure of the IgA basis functions $\varphi_{n,i} = \widehat{\varphi}_{n,i} \circ \Phi_n^{-1}$. Hence, for each time slice Q_n , $n = 1, \dots, N$, the basis functions $\varphi_{n,i}$, $i \in \mathcal{I}_n$, can be rewritten in the form

$$\varphi_{n,i}(x, t) = \phi_{n,i_x}(x) \psi_{n,i_t}(t), \quad \text{with } i_x \in \{1, \dots, N_{n,x}\} \text{ and } i_t \in \{1, \dots, N_{n,t}\},$$

where $\dim(V_{0n}) = N_{n,x}N_{n,t}$. Using this representation in the definition of the bilinear form $a_n(\cdot, \cdot)$, we obtain

$$\begin{aligned}
& \int_{Q_n} \left(\partial_t \varphi_{n,j} (\varphi_{n,i} + \theta_n h_n \partial_t \varphi_{n,i}) + \nabla_x \varphi_{n,j} \cdot \nabla_x \varphi_{n,i} + \theta_n h_n \nabla_x \varphi_{n,j} \cdot \nabla_x \partial_t \varphi_{n,i} \right) dx dt \\
& + \int_{\Sigma_{n-1}} [|\varphi_{n,j}|] \varphi_{n,i} dx \\
& = \left[\int_{\Omega} \phi_{n,j_x} \phi_{n,i_x} dx \right] \left[\int_{t_{n-1}}^{t_n} \partial_t \psi_{n,j_t} (\psi_{n,i_t} + \theta_n h_n \partial_t \psi_{n,i_t}) dt \right] \\
& + \left[\int_{\Omega} \nabla_x \phi_{n,j_x} \cdot \nabla_x \phi_{n,i_x} dx \right] \left[\int_{t_{n-1}}^{t_n} \psi_{n,j_t} (\psi_{n,i_t} + \theta_n h_n \partial_t \psi_{n,i_t}) dt \right] \\
& + \left[\int_{\Omega} \phi_{n-1,k_x} \phi_{n,i_x} dx \right] \left[(\psi_{n,j_t}(t_{n-1}) - \psi_{n-1,k_t}(t_{n-1})) \psi_{n,i_t}(t_{n-1}) \right] \\
& = \mathbf{M}_{n,x}[i_x, j_x] \mathbf{K}_{n,t}[i_t, j_t] + \mathbf{K}_{n,x}[i_x, j_x] \mathbf{M}_{n,t}[i_t, j_t] - \widetilde{\mathbf{M}}_{n,x}[i_x, k_x] \mathbf{N}_{n,t}[i_t, k_t],
\end{aligned}$$

with the standard mass and stiffness matrices wrt to space

$$\begin{aligned}
\mathbf{M}_{n,x}[i_x, j_x] &:= \int_{\Omega} \phi_{n,j_x} \phi_{n,i_x} dx, & \mathbf{K}_x[i_x, j_x] &:= \int_{\Omega} \nabla_x \phi_{n,j_x} \cdot \nabla_x \phi_{n,i_x} dx, \\
\widetilde{\mathbf{M}}_{n,x}[i_x, k_x] &:= \int_{\Omega} \phi_{n-1,k_x} \phi_{n,i_x} dx,
\end{aligned}$$

and the corresponding matrices wrt to time

$$\begin{aligned}
\mathbf{K}_{n,t}[i_t, j_t] &:= \int_{t_{n-1}}^{t_n} \partial_t \psi_{n,j_t} (\psi_{n,i_t} + \theta_n h_n \partial_t \psi_{n,i_t}) dt + \psi_{n,j_t}(t_{n-1}) \psi_{n,i_t}(t_{n-1}), \\
\mathbf{M}_{n,t}[i_t, j_t] &:= \int_{t_{n-1}}^{t_n} \psi_{n,j_t} (\psi_{n,i_t} + \theta_n h_n \partial_t \psi_{n,i_t}) dt, \\
\mathbf{N}_{n,t}[i_t, k_t] &:= \psi_{n-1,k_t}(t_{n-1}) \psi_{n,i_t}(t_{n-1}).
\end{aligned}$$

With this computations, we have shown that the Galerkin matrix \mathbf{L}_h can be rewritten in the block form

$$\mathbf{L}_h = \begin{pmatrix} \mathbf{A}_1 & & & & \\ -\mathbf{B}_2 & \mathbf{A}_2 & & & \\ & & \ddots & \ddots & \\ & & & & -\mathbf{B}_N & \mathbf{A}_N \end{pmatrix},$$

with the matrices $\mathbf{A}_n := \mathbf{M}_{n,x} \otimes \mathbf{K}_{n,t} + \mathbf{K}_{n,x} \otimes \mathbf{M}_{n,t}$ for $n = 1, \dots, N$, and $\mathbf{B}_n := \widetilde{\mathbf{M}}_{n,x} \otimes \mathbf{N}_{n,t}$ for $n = 2, \dots, N$.

Thus, the linear system (15) can sequentially be solved from one time slice Q_{n-1} to the next time slice Q_n , where a linear system with the system matrix \mathbf{A}_n has to be solved. This can be done, for example, by means of an algebraic multigrid method, which was already successfully used for the single patch case

in [11]. More advanced solvers for the linear system (15) are given by space-time multigrid methods, which allow parallelization wrt to space and time. The problem given in (15) perfectly fits into the framework of space-time multigrid methods introduced in [6].

6 Numerical Results

In this section, we demonstrate the proposed method for the spatial computational domain $\Omega = (0, 1)^3$ and $T = 1$, i.e., $Q = (0, 1)^4$. We consider the manufactured solution $u(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3) \sin(\pi t)$ for problem (1). Here, we only show results for the case $p_n = 1$, $n = 1, \dots, N$, i.e., for lowest order splines. We start with an initial space-time mesh consisting of 64 elements in space and one time slice ($N = 1$) which is subdivided into 8 elements. We then apply uniform refinement wrt space, and increase the number of time slices by a factor of two. At the same time, we keep the number of subdivision per time slice constant. For each time slice, we always use the same parameter $\theta_n = 0.2$. Using the results of Section 5, we can generate the linear system (15) very fast. Moreover, we can apply the solver technology given in [11] to solve the linear system in parallel wrt space and time. In detail, we use the space-time multigrid method (1 V -cycle in time and space, and 1 *hypre* algebraic multigrid (AMG) V -cycle in space) as a preconditioner for the GMRES method, and we stop the iterations until a relative residual error of 10^{-8} is reached. In Table 1, we show the convergence of this approach with respect to the $L_2(Q)$ -norm. We observe the optimal convergence rate of 2. The number of cores used for the *hypre* AMG is denoted by c_x , whereas c_t gives the number of cores with respect to time. Overall, we use $c_x c_t$ cores, which is also listed in this table. We also observe quite small iteration numbers. Finally, we can solve the global linear system with 9 777 365 568 unknowns in less than 5 minutes on a massively parallel machine with 131 072 cores. The weak parallel efficiency corresponding to the last two rows of Table 1 is about 50%. This is due to the massive space parallelization of the AMG that is not especially adapted to the problem under consideration. All computations have been performed on the Vulcan BlueGene/Q at Livermore, U.S.A, MFEM.

N	dof per slice	overall dof	$\ u - u_h\ _{L_2(Q)}$	eoc	c_x	c_t	cores	iter	time [s]
1	1 125	1 125	1.8815E-02	-	1	1	1	1	0.04
2	6 561	13 122	4.8619E-03	1.95	1	2	2	9	1.35
4	44 217	176 868	1.2294E-03	1.98	1	4	4	12	18.72
8	323 433	2 587 464	3.0834E-04	2.00	4	8	32	13	58.81
16	2 471 625	39 546 000	7.7092E-05	2.00	32	16	512	15	109.79
32	19 320 201	618 246 432	1.92621E-05	2.00	256	32	8192	16	133.31
64	152 771 337	9 777 365 568	4.81335E-06	2.00	2048	64	131072	18	273.27

Table 1. Convergence results for the space-time IgA as well as iteration numbers and solving times for the parallel space-time multigrid preconditioned GMRES method.

7 Summary and Conclusion

We presented new time-upwind stabilized multi-patch space-time IgA schemes for parabolic IBVP, derived a priori discretization error estimates, and provided fast generation and solution methods, which can be efficiently implemented on massively parallel computers as the first numerical results show. This space-time method can be generalized to more general parabolic evolution problems.

Acknowledgments

The authors gratefully acknowledge the financial support by the Austrian Science Fund (FWF) under the grants NFN S117-03. We also want to thank the Lawrence Livermore National Laboratory for the possibility to perform numerical test on the Vulcan Cluster. In particular, the second author wants to thank P. Vassilevski for the support and the fruitful discussions during his visit at the Lawrence Livermore National Laboratory.

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